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14. ABSTRACT
The vital link between low-energy electron elastic scattering resonances and low-energy chemical reaction dynamics has been fully established, leading to the fundamental understanding of the mechanism driving nanoscale catalysis as well as sensor technology through atomic negative ions. The production of methanol from methane without CO2 emission and water catalysis to peroxide through the use of the atomic Au anion catalyst has been accomplished. Greenhouse gas emissions will be impacted and observational Astronomy will be facilitated.

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Report Title

Final Report: Simulation of Quantum Phenomena in Nanowire Sensors

ABSTRACT

The vital link between low-energy electron elastic scattering resonances and low-energy chemical reaction dynamics has been fully established, leading to the fundamental understanding of the mechanism driving nanoscale catalysis as well as sensor technology through atomic negative ions. The production of methanol from methane without CO2 emission and water catalysis to peroxide through the use of the atomic Au anion catalyst has been accomplished. Greenhouse gas emissions will be impacted and observational Astronomy will be facilitated. Vessels could be lined with nanopaladium or nanogold negative ions to carry drinking water, impacting the weight of a soldier significantly. Industrial furnaces and jet engines could be coated with nanogold or nanosilver negative ion catalysts for the combustion of methane gas without the CO2 emission. A novel mechanism for explaining the matter-antimatter asymmetry of the Universe has also been advanced. The obtained photoabsorption spectrum of the Xe@C60 endohedral fullerene confirms the three main peaks observed in the measured data. This and the knowledge of other giant endohedral fullerenes could impact quantum computing and drug delivery. Our international collaboration has unveiled the fundamental properties of the exotic quantum spin liquid (QSL), formed with such hypothetic particles as fermionic spinons carrying spin 1/2 and no charge; QSL forms a strongly correlated Fermi system located at a fermion condensation quantum phase transition.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received		Paper
01/30/2013	1.00	Alfred Z. Msezane, Zineb Felfli, Kelvin Suggs, Aron Tesfamichael, Xiao-Qian Wang. Gold anion catalysis of methane to methanol, Gold Bulletin, (07 2012): 0. doi: 10.1007/s13404-012-0056-7
02/20/2014	20.00	Alfred Z. Msezane, Zhifan Chen. Off-center effect on the photoabsorption spectra of encapsulated Xe atoms, Physical Review A, (02 2014): 0. doi: 10.1103/PhysRevA.89.025401
02/20/2014	19.00	Zhifan Chen, Alfred Z. Msezane. Photoabsorption spectra of the Ce atom encapsulated inside a C_{82} fullerene, Physical Review A, (10 2013): 0. doi: 10.1103/PhysRevA.88.043423
02/25/2013	2.00	Z Felfli, A Z Msezane and D Sokolovski. Slow electron elastic scattering crosssections for In, Tl, Ga and At atoms, J. Phys. B: At. Mol. Opt. Phys. , (02 2012): 45201. doi:
02/26/2013	3.00	Zhifan Chen and Alfred Z Msezane. Photoabsorption spectrum of theSc3N@C80 molecule, J. Phys. B: At. Mol. Opt. Phys. , (11 2012): 235205. doi:
02/26/2013	4.00	A. S. Baltenkov, S. T. Manson and A. Z. Msezane. A Mathematical Model of Negative Molecular Ion, Proceedings of Dynamic Systems and Applications, (10 2012): 53. doi:
02/26/2013	5.00	Zhifan Chen and A.Z. Msezane. Photoabsorption spectrum of the Xe@C60 endohedral fullerene, Eur. Phys. J. D, (11 2012): 184. doi:
02/26/2013	6.00	Z. F. Chen and A. Z. Msezane. Photoionization of the Xe atom and Xe@C60 molecule, Eur. Phys. J. D, (12 2011): 0. doi:
02/26/2013	7.00	Aron Tesfamichael, Kelvin Suggs, Zineb Felfli, Xiao-Qian Wang, and Alfred Z. Msezane. Atomic Gold and Palladium Negative-Ion Catalysis of Light,2 Intermediate, and Heavy Water to Corresponding Peroxides, J. Phys. Chem. C, (08 2012): 18698. doi:
02/26/2013	8.00	Aron Tesfamichael, Kelvin Suggs, Zineb Felfli,, Xiao-Qian Wang, Alfred Z. Msezane. Atomic gold and palladium negative ion-catalysis of waterto peroxide: fundamental mechanism, J Nanopart. Res., (01 2013): 1333. doi:
02/26/2013	9.00	Zhifan Chen and Alfred Z. Msezane. Effect of C60 giant resonance on the photoabsorption of encaged atoms, Phys Rev A, (10 2012): 63405. doi:
08/21/2013	11.00	V. R. Shaginyan, A. Z. Msezane, K. G. Popov, G. S. Japaridze, V. A. Khodel. Common quantum phase transition in quasicrystals and heavy-fermion metals, Physical Review B, (06 2013): 0. doi: 10.1103/PhysRevB.87.245122
08/21/2013	12.00	Z Felfli, A Z Msezane, D Sokolovski. Elastic scattering of slow electrons from Y, Ru, Pd, Ag and Pt atoms: search for nanocatalysts, Journal of Physics B: Atomic, Molecular and Optical Physics, (07 2011): 0. doi: 10.1088/0953-4075/44/13/135204

08/21/2013 13.00 Z. Felfli, A. Z. Msezane, D. Sokolovski. Complex angular momentum analysis of low-energy electron elastic scattering from lanthanide atoms,
Physical Review A, (04 2010): 0. doi: 10.1103/PhysRevA.81.042707

08/21/2013 14.00 Zineb Felfli, Dmitri Sokolovski, Alfred Z Msezane. Novel mechanism for nanoscale catalysis,
Journal of Physics B: Atomic, Molecular and Optical Physics, (10 2010): 0. doi: 10.1088/0953-4075/43/20/201001

08/21/2013 16.00 A Z Msezane, S T Manson, A S Baltenkov, U Becker. Interference in the molecular photoionization and Young's double-slit experiment,
Journal of Physics B: Atomic, Molecular and Optical Physics, (02 2012): 0. doi: 10.1088/0953-4075/45/3/035202

08/21/2013 17.00 V. R. Shaginyan, A. Z. Msezane, K. G. Popov, G. S. Japaridze, V. A. Stephanovich. Identification of strongly correlated spin liquid in herbertsmithite,
EPL (Europhysics Letters), (03 2012): 0. doi: 10.1209/0295-5075/97/56001

08/21/2013 18.00 K M Aggarwal, F P Keenan, A Z Msezane. Energy levels and radiative rates for transitions in Ti VI,
Physica Scripta, (08 2013): 0. doi: 10.1088/0031-8949/88/02/025302

TOTAL: **18**

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received Paper

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

"Universal behavior of the thermopower of heavy-fermion metals",V. R. Shaginyan, A. Z. Msezane, G. S. Japaridze, K. G. Popov, J. W. Clark, and V. A. Khodel, Phys. Rev. B, Rapid Comm. (Submitted, 2014), arXiv:1410.7299 [cond-mat.str-el]

Number of Presentations: 1.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

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Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received Paper

TOTAL:

Number of Manuscripts:

Books

Received Book

TOTAL:

Received Book Chapter

TOTAL:

Patents Submitted

Patents Awarded

Awards

2011 Elected Fellow of The American Association for the Advancement of Science (AAAS), Physics Division

2013 Nominated Fellow of The Academy of the Sciences of the Developing World, Trieste, Italy

2013 Appointed Member of Advisory Commission of the UNESCO-UNISA Africa Chair in Nanosciences/Nanotechnology, University of South Africa, Pretoria

Alfred Msezane

2013 Entered into ScienceMaker, Library of Congress, a NSF-Sponsored Project

2013-present Appointed Member of Europe-Africa Foundation for Science & Technology

2013-present Appointed Editorial Board Member, Nanoscience & Technology: Open Access

2014 Appointed Member of International Advisory Committee, African Laser Centre Annual Workshop 3-5 Nov. 2014, Moroccan Foundation for Advanced Science, Innovation & Research, Faculty of Sciences, University Mohammed V – Agdal, (FSR)

Graduate Students

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:...... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):...... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:...... 0.00

Names of Personnel receiving masters degrees

NAME
Total Number:

Names of personnel receiving PHDs

NAME
Total Number:

Names of other research staff

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

Summary of Accomplishments: Final Report

The research project has achieved significant results in two main areas:
I. Low-energy electron scattering, leading to a fundamental understanding of nanoscale catalysis through negative ion resonances.
II. Photoabsorption of Xe atoms encapsulated inside fullerenes

The essentials of each area are presented and discussed below; the details are found in the published or to be published (completed) papers

I. Low-energy electron scattering resonances: Catalysts and Sensors

I.1 Overview

The present research has now fully established the vital link between low-energy electron elastic scattering resonances (maxima and minima in the electron elastic scattering total cross sections) and low-energy chemical reaction dynamics. Consequently, the fundamental atomic physics mechanism driving nanoscale catalysis, namely responsible for the oxidation of water to peroxide, has been attributed to the interplay between resonances and Ramsauer–Townsend (R–T) minima that characterize the low-energy electron elastic scattering total cross sections (TCSs) for Au and Pd atoms, along with their large electron affinities (EAs) [1]. Many more chemical reactions, particularly nanocatalysis, including sensor technology, can now be studied and analyzed using the electron–Au scattering TCSs as the benchmark. So, the investigation and delineation of the resonance structures in the TCSs for low-energy electron elastic scattering can now take center stage.

The role of atomic particles and nanoparticles in catalysis continues to attract extensive investigations from both fundamental and industrial perspectives. Recently, our research group has added the novel atomic negative ions to the study of catalysis at the atomic scale by performing transition state calculations using dispersion-corrected density-functional theory for the following reactions: 1) Conversion of H_2O, HDO, and D_2O to H_2O_2, HDO_2, and D_2O_2, respectively using atomic Au^- and atomic Pd^- ion catalysis [2, 3] and 2) Complete and partial oxidation of methane in the absence and presence of the atomic Au^- ion catalyst [4-6]. The fundamental mechanism of negative ion catalysis in the oxidation of water to peroxide catalyzed by the atomic Au^- ion has been attributed to the anionic molecular complex $Au^-(H_2O)_{1,2}$ formation in the transition state, with the atomic Au^- ion breaking up the hydrogen bond strength in the water molecules, permitting the formation of the peroxide in the presence of O_2 usually provided by the support. Similarly, in the conversion of methane to methanol using the atomic Au^- ion catalyst, the anionic molecular complex $Au^-(CH_4)$ formation, weakens the C-H bond in the transition state.

I.2 Tunable Catalysis of Water to Peroxide

In the paper “Tunable Catalysis of Water to Peroxide” [6] we employed a scalable method to investigate the optimization of the catalytic behavior of Au, Ag, Pd, Rh, and Os atomic systems via polarization effects and conclude that anionic atomic systems are optimal and therefore ideal for catalyzing the oxidation of water to peroxide, and that anionic Os is the best candidate among the atomic anions investigated. These results confirm our recent complex angular momentum analysis identifying negative atomic ions as the fundamental mechanism of catalysis at the atomic scale with the implication that the anionic atomic systems are optimal configurations for catalytic behavior [7]. Also important here is the discovery that cationic systems increase the transition energy barrier in the synthesis of peroxide; this could render them important as inhibitors in controlling and regulating catalysis as well as in the design and manufacture of sensors.

In general, these calculations using density functional theory provide insight into the catalytic behavior of higher order dimensional transition metal substrate via ionic tuning of fundamental atomic species, and imply guidance for scale-up approaches. Hence, a plausible theoretical foundation for tailoring and optimizing transition metal substrate identification, processing, and industrial application is inferred. Furthermore, there is an implication that these results may plausibly extend to negatively charged enzymes in biological systems, polymers, and organic substrates, and pose an interesting hypothesis as to whether this is consistent across interdisciplinary systems, reaction types, atomic cluster substrates and ionic solutions. This conclusion should also be applicable to the oxidation of methane to methanol without CO_2 emission, with the anionic Os being the best catalyst. These findings usher in a fundamental atomic theoretical framework for the generation of tunable catalytic systems, with application also to sensor technology.

II. Photoabsorption spectra of Xe atoms encapsulated inside fullerenes

Endohedral fullerenes are not only of scientific interest but also promise important applications in quantum computing, magnetic resonance imaging, nuclear magnetic resonance analysis, drug delivery and sensor technology.

In this section we discuss the confinement resonances of Xe atoms encapsulated inside fullerenes (1) C_{180} and C_{240}, which are close to a sphere and (2) C_{58}, C_{56} and C_{54}, which are deformed from a sphere. The photoabsorption spectra of Xe atoms encapsulated inside fullerenes have been investigated using the time-dependent density-functional theory (TDDFT) and compared for C_{180} and C_{240} with the results of our short range spherical well potential.

II.1 Overview

In the photoionization studies of endohedral fullerenes the most attractive problem is the Xe 4d confinement resonances in the Xe@C60 molecule. The demonstration that in the photoionization of Xe@C60, the 4d giant resonance is distorted significantly when compared with that of the isolated Xe atom [8], has stimulated a number of investigations, including the first experimental discovery of confinement in the photoionization of the 4d subshell of the Xe atom in molecular Xe@C60 [9]. Hitherto for, almost all the studies of the Xe confinement resonances have been focused on the Xe@C60 endohedral fullerene. A recent R-matrix calculation which agreed with the measurement therein [10], as well as a fully relativistic R-matrix calculation [11] used a delta-type model potential. However, the R-matrix calculation used in the measurement in [10] has been criticized severely [12]. Our short range spherical well potential [13] gave better results compared to the δ-like potential with respect to the measurement [9]. Most important here, our calculation using the TDDFT with pseudopotential [14] can evaluate the photoabsorption spectra when the Xe atom is located off the center. A recent study indicated that the photoionization cross section of the encaged Xe atom is very sensitive to the position of the Xe atom [15]. The confinement resonances can be observed only if the Xe atom is located at about 0.3 ˚A around the center. Unfortunately, current experimental techniques can't determine the location of the Xe atom inside the C60. This is the main source of controversy among the theoretical calculations which aim at reproducing the measurements.

II.2 Results

A. For the photoabsorption spectra of Xe atoms encapsulated inside C180 and C240 we found:

1) The Xe-C180 and Xe-C240 binding energies along some high symmetry directions showed the possibility of other Xe positions. For the Xe@C240 molecule the changes in the Xe-C240 binding energies with the off-center distance of the Xe atom demonstrates two minima for the Xe-C240; one is at the center of the cage, while the other is near r = 3.2 ˚A.

2) It is noted that if r is less than 3.4 ˚A the Xe-C240 binding energies are all negative. This implies that if the Xe atom has enough kinetic energy it should move rather freely within a spherical ball with the radius of r < 3.4 ˚

3) The main features of the confinement resonances for the Xe atoms inside C180 and C240 may be predicted by our simple empirical formula relating the location of a confinement peak to the radius of a fullerene. If the radius of a fullerene equals an integer (≥ 2) × the half wave length of the photoelectron, then at this photon energy we may be able to observe a confinement peak.

4) The agreement between the two methods (the TDDFT and the short range potential well) is reasonably good; both methods demonstrate the significant distortion of the Xe 4d giant resonance, consistent with the prediction in [8].

B. For the Xe atom inside C58, which has similar confinement resonances as those of the Xe atom inside C60, the spectra of Xe inside C56 and C54 are completely different from that of the Xe inside C60 which are characterized by confinement resonances of the Xe@C60 molecule. This is related to the larger deformation parameters of the C56 and C54. It is concluded that the quantum confinement resonances will be destroyed if the shape of the fullerene is deformed significantly from a sphere. The appearance of additional peaks in the spectra of giant endohedral fullerenes can be understood as follows. The radii for the C180 and C240 are respectively, 6.16 and 7.10 A from our calculations [16]. They are much larger than the 3.5 ˚A radius of the C60. Therefore, their extended space allows for the generation of more standing waves.

Technology Transfer

Quantum simulation of novel nano materials and catalysis

Reporting Period: 19 May, 2011 to 19 December, 2014

Participants:
Faculty: Drs. A. Z. Msezane, Xiao-Qian Wang and Zhifan Chen
Students, Graduate: Aron Tesfamichael and Kelvin Suggs
Students, Undergraduate: Filmon Kiros

Honor: Dr. Msezane was

2011 Elected Fellow of The American Association for the Advancement of Science (AAAS), Physics Division
2013 Nominated Fellow of The Academy of the Sciences of the Developing World, Trieste, Italy
2013 Appointed Member of Advisory Commission of the UNESCO-UNISA Africa Chair in Nanosciences/Nanotechnology, University of South Africa, Pretoria
2013 Entered into ScienceMaker, Library of Congress, a NSF-Sponsored Project
2013- Appointed Member of Europe-Africa Foundation for Science & Technology
2013- Appointed Editorial Board Member, Nanoscience & Technology: Open Access
2014 Appointed Member of International Advisory Committee, African Laser Centre Annual Workshop 3-5 Nov. 2014, Moroccan Foundation for Advanced Science, Innovation & Research, Faculty of Sciences, University Mohammed V – Agdal, (FSR)

Abstract

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3) The main features of the confinement resonances for the Xe atoms inside C180 and C240 may be predicted by our simple empirical formula relating the location of a confinement peak to the radius of a fullerene. If the radius of a fullerene equals an integer (≥ 2) × the half wave length of the photoelectron, then at this photon energy we may be able to observe a confinement peak.

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References

[1] A. Z. Msezane, Z. Felfli and D. Sokolovski, Novel mechanism for nanoscale catalysis: J. Phys. B **43**, 201001 (2010).

[2] A. Z. Msezane, Z. Felfli, A. Tesfamichael, K. Suggs, and X. – Q. Wang, Gold anion catalysis of methane to methanol: Gold Bulletin, **3** (45), 127-135 (2012).

[3] "Methane Oxidation to Methanol without CO_2 Emission: Catalysis by Atomic Negative Ions", Aron Tesfamichael, Kelvin Suggs, Zineb Felfli, and Alfred Z. Msezane, arXiv:1403.0597 [physics.chem-ph] (2014).

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[7] "Tunable Catalysis of Water to Peroxide with Anionic, Cationic, and Neutral Atomic Au, Ag, Pd, Rh, and Os", Kelvin Suggs, Filmon Kiros, Aaron Tesfamichael, Zineb Felfli, Alfred Z. Msezane, arXiv:1410.4893v1 [physics.atm-clus](2014)

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II. OUR PUBLICATIONS (Yellow-highlighted acknowledge grant)

[1] "Elastic scattering of slow electrons from Y, Ru, Pd, Ag and Pt atoms: Search for nanocatalysts", Z. Felfli, A.Z. Msezane and D. Sokolovski, J. Phys. B **44**, 135204 (2011)

[2] "Complex angular momentum analysis of low-energy electron elastic scattering from lanthanide atoms", Z. Felfli, A.Z. Msezane and D. Sokolovski, Phys. Rev. A **81**, 042707 (2010)

[3] "Novel mechanism for nanoscale catalysis", A.Z. Msezane, Z. Felfli and D. Sokolovski, J. Phys. B **43**, 201001 (2010) (FAST TRACK)

[4] "Negative ion resonances proposed as mechanism for nanoscale catalysis", A.Z. Msezane, Z. Felfli and D. Sokolovski, *Europhys. News* **41**, 11 (2010)

[5] "Atomic Au and Pd Negative Ion-Catalysis of Water to Peroxide: Fundamental Mechanism", Aron Tesfamichael, Kelvin Suggs, Zineb Felfli, Xiao-Qian Wang and Alfred Z. Msezane, J. Nanoparticle Research **15**, 1333 (2013), DOI 10.1007/s11051-012-1333-3

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[8] "Gold anion catalysis of methane to methanol**",** Alfred Z. Msezane, Zineb Felfli, Aron Tesfamichael, Kelvin Suggs, and Xiao-Qian Wang, Gold Bulletin, DOI10.1007/s13404-012-0056-7

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[18] "Innershell Photoionization of Atomic Chlorine," W. C. Stolte, Z. Felfli, R. Guillemin, G. Ohrwall, S.–W. Yu, J. A. Young, D. W. Lindle, T. W. Gorczyca, N. C. Deb, S. T. Manson, A. Hibbert, and A. Z. Msezane, Phys. Rev. A **88**, 053425 (2013), DOI: http://dx.doi.org/10.1103/PhysRevA.88.053425

[19] " Off-center effect on the photoabsorption spectra of encapsulated Xe atoms", Zhifan Chen and Alfred Z. Msezane, Phys. Rev. A **89**, 025401 (2014), DOI: http://dx.doi.org/10.1103/PhysRevA.89.025401

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PAPERS SUBMITTED 2014

[1] "Tunable Catalysis of Water to Peroxide with Anionic, Cationic, and Neutral Atomic Au, Ag, Pd, Rh, and Os", Kelvin Suggs, Filmon Kiros, Aaron Tesfamichael , Zineb Felfli and Alfred Z. Msezane, ,JJJJJ, (2014), http://arxiv.org/abs/1410.4893

[2] "Intersection of low-energy electron-atom scattering and photodetachment of negative Ions", Zineb Felfli and Alfred Z. Msezane , Phys. Rev. A (Submitted, November, 2014), http://arxiv.org/abs/1403.0559

[3] "Photoabsorption spectra of Xe atoms encapsulated inside fullerenes", Zhifan Chen and Alfred Z Msezane, Euro. Phys. J. D (At Press8, 2014)

[4] "Comment on Experimental Studies of Os^-: Observation of a Bound-Bound Electric Dipole Transition in an Atomic Negative Ion", Zineb Felfli, Filmon Kiros, Kelvin Suggs and Alfred Z. Msezane, http://arxiv.org/pdf/1208.1522

[5] "Resonances in low-energy electron elastic scattering from Os atom: New electron affinity", Zineb Felfli, Filmon Kiros and Alfred Z. Msezane, Phys. Rev. A (To be Submitted, 2014)

[**6**] "Methane Oxidation to Methanol without CO_2 Emission: Catalysis by Atomic Negative Ions", Aron Tesfamichael, Kelvin Suggs, Zineb Felfli, and Alfred Z. Msezane, Chem. Phys. Lett. Submitted (2014)

PAPERS Published In PROCEEDINGS

[1] "Slow electron scattering from Ag, Pd, Pt, Ru and Y atoms: Search for nanocatalysts", A. Z. Msezane, Z. Felfli, and D. Sokolovski, Journal of Physics: Conference Series **388**, 042002 (2012)

[2] "Near-threshold electron elastic scattering cross sections for Ta, W, Re, Mo, Tc and Rh atoms: Determination of electron affinities and Ramsauer-Townsend minima", Zineb Felfli, Alfred Msezane, and Dmitri Sokolovski, Journal of Physics: Conference Series **488,** 042019 (2014)

SPECIAL PUBLICATION (Invited)

2014 "Nelson Mandela's Leadership", Alfred Z. Msezane and Sekazi K. Mtingwa, The Back Page - American Physical Society **,** http://www.aps.org/publications/apsnews/201405/backpage.cfm

III. EVALUATED (April 2012 – November 2014):

1. Research Proposals for the African Laser Centre, Pretoria, South Africa, November , 2012
2. Research Proposal for The National Academies for the Sciences, May, September, December, 2012
3. Fellowship Applicants for PRINTPACK, Inc., Atlanta, April 22, 2012
4. Research Proposals for The National Academies of the Sciences, Irvine, CA, March 9-12, 2013
5. Fellowship Applicants for PRINTPACK, Inc., Atlanta, April 25, 2013
6. Manuscripts for various physics journals for publication and research proposals for various agencies (J. Phys. B; Can. J. Phys.; Indian J. Phys. ; Surface Science Reviews; Phys. Rev.; Euro Phys. J., Computer Physics Communications, Journal of Electron Spectroscopy and Related Phenomena, DOE Research Proposal)
7. Fellowship Applicants for PRINTPACK, Inc., Atlanta, April 28, 2014
8. Research Proposals for the African Laser Centre, CSIR, Pretoria, South Africa, November 2013 at the Cradle of Humankind

9. Research Proposals for the African Laser Centre, CSIR, Pretoria, South Africa, November 2014 in Durban .

IV. CONFERENCE PRESENTATIONS (Acknowledging Grant), 2012 - 2014

43rd Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics, June 4- 8, 2012 Anaheim, California

1. "Photoabsorption spectrum of the Xe@C60 endohedral fullerene", Zhifan Chen and Alfred Z Msezane, Bull. Am. Phys. Soc. **57**, 39, D1 19 (2012)
2. "Interchannel coupling effects in multi-channel potential scattering", D. Sokolovski, Z. Felfli and A.Z. Msezane, Bull. Am. Phys. Soc. **57**, 105, K1 49 (2012)
3. "Resonances in slow electron collisions with In, Tl, Ga and At atoms: Accurate electron affinities", Z. Felfli, A.Z. Msezane and D. Sokolovski, Bull. Am. Phys. Soc. **57**, 163, Q1 47 (2012)
4. "Atomic Au and Pd Negative-Ion Catalysis of H_2O, HDO and D_2O to Corresponding Peroxides", Aron Tesfamichael, Kelvin Suggs, Zineb Felfli, Xiao-Qian Wang and Alfred Z. Msezane, Bull. Am. Phys. Soc. **57**, 180, Q1 150 (2012)
5. "Energy levels and radiative rates for transitions in Ti VI", K. Aggarwal, F. Keenan and A. Z. Msezane, Bull. Am. Phys. Soc. **57**, 180, K1 10 (2012)

23rd International Conference on Atomic Physics (ICAP 2012), Ecole Polytechnique in Palaiseau (France) July 23-27, 2012

1. "Large scale CIV3 calculations of fine-structure energy levels and lifetimes in Co XIV" , G. P. Gupta and A. Z. Msezane

2012 Social Sciences Research Conference "The re-emergence of astronomy in Africa – a transdisciplinary interface of knowledge systems"

Venue: Cradle of Mankind Conference Centre, Maropeng, South Africa
Date: 10 and 11 September 2012

***Invited Talk*: "**Bring our heads together something happens**", Alfred Z. Msezane**

2013 Joint Meeting of the APS Division of Atomic, Molecular & Optical Physics and the CAP Division of Atomic, Molecular & Optical Physics, Canada, Volume 58, Number 6

Monday–Friday, June 3–7, 2013; Quebec City, Canada

Bulletin of The American Physical Society, Volume 58, Number 6
D1.00018 : Negative-Ion Catalysis of Methane to Methanol without CO2 Emission
Tesfamichael, K. Suggs, Z. Felfli and A.Z. Msezane, Bull. Am. Phys. Soc. **58**, 40 (2013)
D1.00101 : Off center effect on the photoabsorption spectrum of the Xe@C60 endohedral fullerene, Zhifan Chen and Alfred Z. Msezane, Bull. Am. Phys. Soc. **58**, 53 (2013)
D1.00103 : Photoabsorption spectrum of the Ce@C82 endohedral fullerene
Zhifan Chen and Alfred Z. Msezane, Bull. Am. Phys. Soc. **58**, 54 (2013)

K1.00125 : Low-energy electron elastic scattering from Os atom: New electron affinity
Z. Felfli, F. Kiros and A.Z. Msezane, Bull. Am. Phys. Soc. **58**, 119 (2013)

Q1.00088 : Inner-shell Photoionization of Atomic Chlorine: Experiment and Theory
W.C. Stolte, Z. Felfli, A.Z. Msezane, R. Guillemin, G. Ohrwall, S.-W. Yu, J.A. Young, D.W. Lindle, T.W. Gorczyca, N.C. Deb, A. Hibbert and S.T. Manson, Bull. Am. Phys. Soc. **58**, 169 (2013)

XXVII International Conference on Photonic, Electronic and Atomic Collisions 24-30 July, 2013, Lanzhou, China

1. "Off center effect on the photoabsorption spectrum of the Xe@C60 endohedral fullerene", Zhifan Chen, Alfred Z Msezane, ICPEAC2013, p. 16830
2. "Photoabsorption spectrum of the Ce@C82 endohedral fullerene", Zhifan Chen, Alfred Z Msezane, ICPEAC2013, p. 16831
3. "Fine-structure energy levels and radiative rates in Si-like Cobalt", G. P. Gupta, and A. Z. Msezane, ICPEAC2013, p. 16899
4. "Fine-structure energy levels, oscillator strengths and lifetimes in Al-like Chromium", G. P. Gupta and A. Z. Msezane , ICPEAC2013, p. 16890
5. "Near-threshold electron elastic scattering cross sections for Ta, W, Re, Mo, Tc and Rh atoms: Determination of electron affinities and Ramsauer-Townsend minima", Zineb Felfli, Alfred Msezane, and Dmitri Sokolovski, ICPEAC2013, p. 18216

VI International Symposium "Atomic Cluster Collisions" Wuhan-Chongqing, China 18-23 July, 2013

Invited Talk

"Photoabsorption spectra of atoms encaged inside a fullerene", Zhifan Chen and Alfred Z. Msezane, page 30

2013 Meeting of the Atomic, Molecular and Optical Sciences Program Office of Basic Energy Sciences U.S. Department of Energy, Bolger Center, Potomac, Maryland October 27-30, 2013

Invited Talk

"Electron/Photon Interactions with Atoms/Ions"

LAM 10 INTERNATIONAL WORKSHOP: OPTICS PHOTONICS AND LASERS IN SCIENCE AND TECHNOLOGY FOR SUSTAINABLE DEVELOPMENT

LAUNCHING OF THE AFRICAN OPTICS and PHOTONICS SOCIETY

University Cheikh Anta Diop of Dakar, Dakar, Senegal, 13-18 January 2014

Invited Talk

"Confinement and fullerene plasmon resonances and off-center effect in photoabsorption spectra of endofullerenes: TDDFT Investigations", Zhifan Chen and Alfred Z. Msezane

45th Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics, June 2-6, 2014, Madison, Wisconsin Volume 59, Number 8

1. Q1.00144 The quantum confinement resonances of a Xe atom encapsulated inside fullerenes, Zhifan Chen and A. Z. Msezsane, Bulletin of the American Physical Society **59**, Q1 144 (2014)

2. Q1.00145 The photoabsorption spectra of a Xe atom encapsulated inside C$_{54}$, C$_{56}$, and C$_{58}$ fullerenes, Zhifan Chen and A. Z. Msezsane, Bulletin of the American Physical Society **59**, Q1 145 (2014)

VII. Research Grants, Active (2009 - 2014)

1. **“Electron/Photon Interactions with Atoms/Ions”**
   U.S. DOE Fundamental Interactions Branch, Office of Science
   Period: April 01, 2013 – March 31, 2016

2. **“Research and Engineering Apprenticeship Program (REAP)”**
   Academy of Applied Sciences (ARO) (for High School Students)
   Period: (Annual, Since 1983)
   June 01, 2013 – December 31, 2013

3. **“Simulation of Quantum Phenomena in Nanoscale Biosensors---Bio-Inspired Sciences”**
   U.S. Army (DOD)
   Period: April, 2011 – May, 2014

4. **“Resonances in low-energy electron scattering from atoms relevant to BEC, atmospheric and astrophysical environments and photoionization of positive ions”**
   Air Force Office of Scientific Research, AFOSR
   Period: 09/15/2009 - 08/31/2012
   .

5. **Received 20,000 Supercomputing Units of time from DOE for use on the NERSC Supercomputers**.
   U.S. DOE Basic Energy Sciences
   Period: March 1, 2012 – February 28, 2014

High School Students (Summer, 2013):

1. Kieran Merritt
2. Alexis Weeks
3. Carl Melton
4. Nathaniel Cooper
5. Jasmine Pope
6. Kenisha Pope
7. Ronald L. Braithwaite II

High School Students (Summer, 2014):

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